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L31           8 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L29 OR L30


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L31  ANSWER 1 OF 8  HCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2008:1339565  HCAPLUS  Full-text
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DOCUMENT NUMBER: 149:509677
TITLE: Methods and compositions for stem cell self-renewal, particularly hematopoietic stem cell (HSC), by modulating PTEN and Wnt pathways
INVENTOR(S): Perry, John M.; Li, Linheng; Grindley, Justin C.
PATENT ASSIGNEE(S): Stowers Institute for Medical Research, USA
SOURCE: PCT Int. Appl., 110pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008133904	A1	20081106	WO 2008-US5230	20080423

W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2007-926065P P 20070423
US 2008-66693P P 20080222

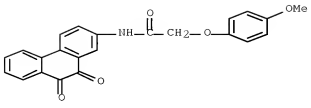
ED Entered STN: 07 Nov 2008

AB The present invention relates to methods for expanding a stem cell population without significant stem cell differentiation by modulating a PTEN phosphatase pathway and a Wnt pathway. More particularly, the invention relates, to methods and compns. for expanding a stem cell population, particularly a hematopoietic stem cell (HSC) population obtained from peripheral blood, cord blood, or bone marrow. The expanded HSC population comprises cells with a phenotype consisting of CD34-, CD34+/CD38-Thy1+/CD90+/Kit-/Lin-/CD133+/VEGFR2+, CD150+/CD48-/CD244-, CD150-/CD48-/CD244+, CD150-/CD48+/CD244+, and combinations thereof. In one embodiment the invention provides a kit for expanding HSC population for subsequent transplantation into a patient in need thereof. The kit comprises a PTEN inhibitor, a GSK-3β (glycogen synthase kinase 3β) inhibitor, and instructions for the use of the inhibitors. It was demonstrated, that loss of PTEN with constitutively active β-catenin leads to HSC expansion with loss of early hematopoietic progenitors. It was also demonstrated, that ex vivo pharmacol. manipulation of the PTEN/Akt and Wnt/β-catenin signaling pathways cooperatively drive functional HSC expansion.

IT 867376-02-1, SF 1751
(reversible PTEN inhibitor; methods and compns. for stem cell self-renewal, particularly hematopoietic stem cell (HSC), by modulating PTEN and Wnt pathways)

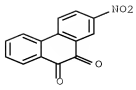
RN 867376-02-1 HCAPLUS

CN Acetamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-2-(4-methoxyphenoxy)- (CA INDEX NAME)



CC 13-6 (Mammalian Biochemistry)
Section cross-reference(s): 3, 9, 63
IT 517-89-5, Shikonin 12179-38-3D, derivs. 867376-02-1, SF 1751
(reversible PTEN inhibitor; methods and compns. for stem cell self-renewal, particularly hematopoietic stem cell (HSC), by modulating PTEN and Wnt pathways)
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

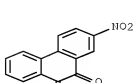
L31 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:1243425 HCAPLUS Full-text
DOCUMENT NUMBER: 149:524585
TITLE: Structure-Based Virtual Screening and Biological Evaluation of Mycobacterium tuberculosis Adenosine 5'-Phosphosulfate Reductase Inhibitors
AUTHOR(S): Cosconati, Sandro; Hong, Jiyoung A.; Novellino, Ettore; Carroll, Kate S.; Goodsell, David S.; Olson, Arthur J.
CORPORATE SOURCE: Department of Molecular Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Journal of Medicinal Chemistry (2008), 51(21), 6627-6630
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 16 Oct 2008
AB Tuberculosis is among the world's deadliest infectious diseases. APS reductase catalyzes the first committed step in bacterial sulfate reduction and is a validated drug target against latent tuberculosis infection. We performed a virtual screening to identify APSR inhibitors. These inhibitors represent the first non-phosphate-based mols. to inhibit APSR. Common chemical features lay the foundation for the development of agents that could shorten the duration of chemotherapy by targeting the latent stage of TB infection.
IT 604-95-5
(structure-based screening and evaluation of M. tuberculosis APSR inhibitors)
RN 604-95-5 HCAPLUS
CN 9,10-Phenanthrenedione, 2-nitro- (CA INDEX NAME)



CC 1-3 (Pharmacology)
IT 604-95-5 6942-44-5 13287-73-5 58160-29-5 113104-25-9
500576-09-0 501687-72-5 820999-41-5 873058-04-9 1073524-06-7
(structure-based screening and evaluation of M. tuberculosis APSR inhibitors)
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1167266 HCAPLUS Full-text
DOCUMENT NUMBER: 147:514411
TITLE: Planarity and Constraint of the Carbonyl Groups in 1,2-Diones Are Determinants for Selective Inhibition of Human Carboxylesterase 1
AUTHOR(S): Hyatt, Janice L.; Wadkins, Randy M.; Tsurkan, Lyudmila; Hicks, Latorya D.; Hatfield, M. Jason; Edwards, Carol C.; Ross, Charles R., II; Cantalupo, Stephanie A.; Crundwell, Guy; Danks, Mary K.; Guy, R. Kip; Potter, Philip M.
CORPORATE SOURCE: Department of Molecular Pharmacology, St. Jude Children's Research Hospital, Memphis, TN, 38105, USA
SOURCE: Journal of Medicinal Chemistry (2007), 50(23), 5727-5734
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:514411
ED Entered STN: 17 Oct 2007
AB Carboxylesterases (CE) are ubiquitous enzymes responsible for the detoxification of xenobiotics, including numerous clin. used drugs. Therefore, the selective inhibition of these proteins may prove useful in modulating drug half-life and bioavailability. Recently, we identified 1,2-diones as potent inhibitors of CEs, although little selectivity was observed in the inhibition of either human liver CE (hCE1) or human intestinal CE (hiCE). In this paper, we have further examined the inhibitory properties of ethane-1,2-diones toward these proteins and determined that, when the carbonyl oxygen atoms are cis-coplanar, the compds. demonstrate specificity for hCE1. Conversely, when the dione oxygen atoms are not planar (or are trans-coplanar), the compds. are more potent at hiCE inhibition. These properties have been validated in over 40 1,2-diones that demonstrate inhibitory activity toward at least one of these enzymes. Statistical anal. of the results confirms the correlation ($P < 0.001$) between the dione dihedral angle and the preferential inhibition of either hiCE or hCE1. Overall, the results presented here define the parameters necessary for small mol. inhibition of human CEs.
IT 604-95-5
(Planarity and Constraint of the Carbonyl Groups in 1,2-Diones Are

Determinants for Selective Inhibition of Human Carboxylesterase 1)
RN 604-95-5 HCAPLUS
CN 9,10-Phenanthrenedione, 2-nitro- (CA INDEX NAME)



CC 1-3 (Pharmacology)
Section cross-reference(s): 25, 27, 28
IT 82-86-0, Acenaphthoquinone 84-11-7, 9,10-Phenanthrenedione
134-81-6, Benzil 524-42-5, 1,2-Naphthoquinone 604-95-5
951-88-2, 1,2-Dicyclohexylethane-1,2-dione 1226-42-2 2103-62-0
2132-59-4 2767-84-2, (+/-)-Camphorquinone 3363-97-1 4290-72-6
4746-81-0, Mesitil 6067-45-4 6373-11-1, 1,2-Aceanthrylenedione
6706-92-9 16214-27-0, 1,2-Indandione 24243-31-0,
Benzo[1,2-b:4,3-b']dithiophene-4,5-dione 27471-02-9 40261-88-9
65938-98-9, Benzo[h]quinoline-5,6-dione
(Planarity and Constraint of the Carbonyl Groups in 1,2-Diones Are Determinants for Selective Inhibition of Human Carboxylesterase 1)
REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1123765 HCAPLUS Full-text
DOCUMENT NUMBER: 143:405906
TITLE: Preparation of (heteroaryl) amides and hydrazides as inhibitors of phosphatase located on chromosome 10 (PTEN).
INVENTOR(S): Garlich, Joseph R.; Durden, Donald L.; Georgiadis, Taxiarchis M.; Su, Jingdong; Peng, Xiaodong; Smith, Tim C.
PATENT ASSIGNEE(S): Semafore Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005097119	A2	20051020	WO 2005-US11626	20050406
WO 2005097119	A3	20060126		

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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2563316	A1	20051020	CA 2005-2563316		20050406
EP 1755574	A2	20070228	EP 2005-763900		20050406
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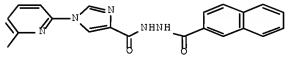
JP 2007532552	T	20071115	JP 2007-507462		20050406
US 20070203098	A1	20070830	US 2006-599748		20061006
PRIORITY APPLN. INFO.:			US 2004-559802P	P	20040406
			US 2004-590043P	P	20040720
			US 2004-625871P	P	20041108
			WO 2005-US11626	W	20050406

OTHER SOURCE(S): CASREACT 143:405906
ED Entered STN: 20 Oct 2005
GI

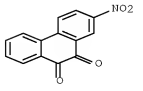


I

AB A method of protecting a patient from ≥1 treatments that trigger apoptosis comprises administration of a pharmaceutically acceptable amount of a PTEN inhibitor. Thus, 1-(6-methyl-2-pyridinyl)-1H-imidazole-4-carbohydrazide was stirred overnight with 2-naphthoyl chloride and Et3N in CH2Cl2 to give title compound (I). I gave 41-43% inhibition of PTEN at 250 μM.

IT 604-95-5P 36043-49-9P 345630-42-4P
860207-88-1P 867376-01-0P 867376-02-1P
867376-03-2P 867376-04-3P 867376-07-6P
867376-10-1P 867376-12-3P 867376-13-4P
867376-14-5P 867376-15-6P 867376-18-9P
867376-20-3P 867376-29-2P 867376-34-9P
867376-35-0P
(preparation of (heteroaryl) amides and hydrazides as inhibitors of phosphatase located on chromosome 10 (PTEN))

RN 604-95-5 HCAPLUS
CN 9,10-Phenanthrenedione, 2-nitro- (CA INDEX NAME)



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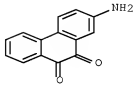

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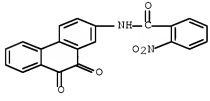

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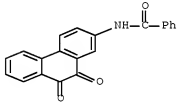

RN 867376-01-0 HCAPLUS
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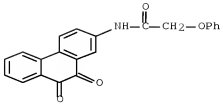

RN 867376-02-1 HCAPLUS
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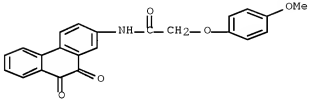

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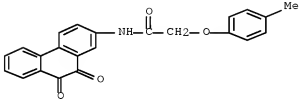

RN 867376-04-3 HCAPLUS
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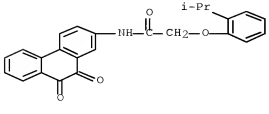

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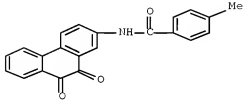

RN 867376-10-1 HCAPLUS
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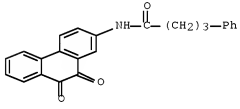
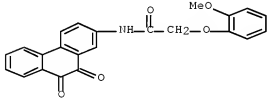
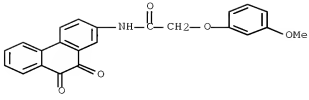


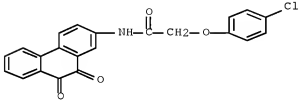
RN 867376-12-3 HCAPLUS
CN Acetamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-2-(2-methoxyphenoxy)- (CA INDEX NAME)



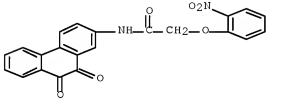
RN 867376-13-4 HCAPLUS
CN Acetamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-2-(3-methoxyphenoxy)- (CA INDEX NAME)



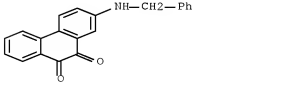
RN 867376-14-5 HCAPLUS
CN Acetamide, 2-(4-chlorophenoxy)-N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)- (CA INDEX NAME)



RN 867376-15-6 HCAPLUS
CN Acetamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-2-(2-nitrophenoxy)- (CA INDEX NAME)

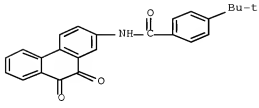


RN 867376-18-9 HCAPLUS
CN 9,10-Phenanthrenedione, 2-[(phenylmethyl)amino]- (CA INDEX NAME)

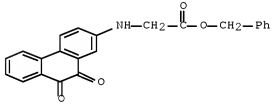


RN 867376-20-3 HCAPLUS

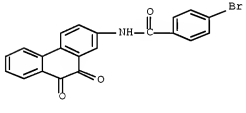
CN Benzamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-4-(1,1-dimethylethyl)- (CA INDEX NAME)



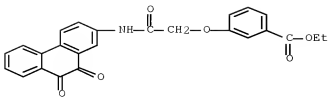
RN 867376-29-2 HCAPLUS
CN Glycine, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-, phenylmethyl ester (CA INDEX NAME)



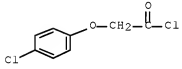
RN 867376-34-9 HCAPLUS
CN Benzamide, 4-bromo-N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)- (CA INDEX NAME)



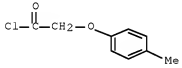
RN 867376-35-0 HCAPLUS
CN Benzoic acid, 3-[2-[(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)amino]-2-oxoethoxy]-, ethyl ester (CA INDEX NAME)



IT 4122-68-3 15516-47-9
(preparation of (heteroaryl) amides and hydrazides as inhibitors of phosphatase located on chromosome 10 (PTEN))
RN 4122-68-3 HCAPLUS
CN Acetyl chloride, 2-(4-chlorophenoxy)- (CA INDEX NAME)



RN 15516-47-9 HCAPLUS
CN Acetyl chloride, 2-(4-methylphenoxy)- (CA INDEX NAME)



IC ICM A61K031-44
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
IT 604-95-5P 36043-49-9P 43100-25-0P 146903-18-6P
162086-14-8P 220965-34-4P 303092-45-7P 345630-40-2P
345630-42-4P 376383-76-5P 458553-48-5P 477847-81-7P
478257-76-0P 511518-73-3P 547730-75-6P 650620-84-1P
774184-51-9P 860207-88-1P 867339-05-7P 867375-71-1P
867375-74-4P 867375-77-7P 867375-78-8P 867375-79-9P
867375-82-4P 867375-88-0P 867375-89-1P 867375-90-4P
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867376-29-2P 867376-33-8P 867376-34-9P
867376-35-0P 867376-36-1P 867376-37-2P 867376-38-3P
867376-39-4P
(preparation of (heteroaryl) amides and hydrazides as inhibitors of phosphatase located on chromosome 10 (PTEN))

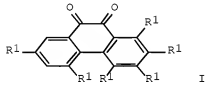
IT 79-04-9 95-54-5, 1,2-Benzenediamine, reactions 98-09-9, Benzenesulfonyl chloride 98-59-9, Tosyl chloride 98-74-8, 4-Nitrobenzenesulfonyl chloride 122-04-3, 4-Nitrobenzoyl chloride 122-59-8 452-58-4, 2,3-Pyridinediamine 496-72-0 586-75-4 610-14-0 619-05-6 694-83-7, 1,2-Diaminocyclohexane 701-99-5, Phenoxyacetyl chloride 874-60-2 939-97-9, 4-tert-Butylbenzaldehyde 1072-84-0, 4-Imidazolecarboxylic acid 1710-98-1, 4-tert-Butylbenzoyl chloride 1821-12-1, 4-Phenylbutyric acid 1878-49-5 2243-83-6, 2-Naphthoyl chloride 2687-25-4 2905-27-3 3282-30-2 4122-68-3 4755-77-5 5271-67-0, 2-Thiophenecarbonyl chloride 5315-25-3, 2-Bromo-6-methylpyridine 5437-45-6 13754-19-3, 4,5-Pyrimidinediamine 15084-51-2, 4-tert-Butylbenzenesulfonyl chloride 15516-47-9 16629-19-9, 2-Thiophenesulfonyl chloride 17325-26-7, Methyl imidazole-4-carboxylate 18496-54-3, 4-Phenylbutanoyl chloride 20142-87-4 40926-73-6 85397-21-3 106967-74-2 1042674-31-6 1042675-60-4
(preparation of (heteroaryl) amides and hydrazides as inhibitors of phosphatase located on chromosome 10 (PTEN))

L31 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:472654 HCAPLUS Full-text
DOCUMENT NUMBER: 135:61559
TITLE: Preparation of phenanthrene-9,10-dione derivatives as CD45 inhibitors
INVENTOR(S): Chapdelaine, Marc Jerome; Knappenberger, Katherine; Steelman, Gary; Suchard, Suzanne; Sygowski, Linda; Urbanek, Rebecca; Veale, Chris Allan
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001046125	A2	20010628	WO 2000-GB4854	20001218
WO 2001046125	A3	20020117		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1242363	A2	20020925	EP 2000-985603	20001218
EP 1242363	B1	20051102		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003518085	T	20030603	JP 2001-547036	20001218

AT 308512	T	20051115	AT 2000-985603		20001218
US 20030207812	A1	20031106	US 2002-168758		20021125
PRIORITY APPLN. INFO.:			US 1999-172788P	P	19991221
			WO 2000-GB4854	W	20001218

OTHER SOURCE(S): MARPAT 135:61559
ED Entered STN: 29 Jun 2001
GI



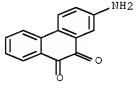
I

AB Substituted phenanthrene-9,10-diones I [R1 at each occurrence is independently selected from H, halogen, NH2, NO2, NHCOR2, CONHR2, Ar, (CH2)nCH(CO2H)R3, COR3, NHCOCH2CH(CO2H)NHR4 and NR52, where R2 = (un)substituted (C1-C4)alkyl, (C1-C8)alkylCO2H or alkyl esters, Ph; n = 1-8; Ar = 3-thienyl, 2-benzofuranyl, 1-naphthyl, 1,3-benzodioxan-5-yl, or (un)substituted phenyl; R3 = certain N-linked oligopeptides; R4 = certain C-linked oligopeptides; R5 = H, tosyl (with provisos)] were prepared for the treatment of T cell mediated conditions such as autoimmune diseases and organ graft rejection. Thus, 9,10-dioxophenanthren-3-ylcarbonyl-Glu-Gln-Pro-Gln-Pro-OH was prepared by the solid-phase method and assayed for biol. activity (pNPP, lck, and T cell proliferation IC50s are 0.6, 2.4, and >30 μM, resp. and CC50 is >30 μM).

IT 36043-49-9P
(preparation of phenanthrenedione derivs. as CD45 inhibitors)

RN 36043-49-9 HCAPLUS

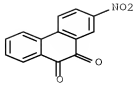
CN 9,10-Phenanthrenedione, 2-amino- (CA INDEX NAME)



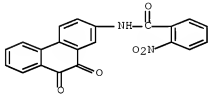
IT 604-95-5P 345630-42-4P
(preparation of phenanthrenedione derivs. as CD45 inhibitors)

RN 604-95-5 HCAPLUS

CN 9,10-Phenanthrenedione, 2-nitro- (CA INDEX NAME)



RN 345630-42-4 HCAPLUS
CN Benzamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-2-nitro- (CA INDEX NAME)



IC ICM C07C237-00
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 15, 25
IT 604-94-4P 32060-67-6P 32155-34-3P 36043-49-9P
47194-23-0P 49546-41-0P 51789-39-0P 53622-33-6P 109497-01-0P
345631-37-0P 345631-41-6P 345631-42-7P
(preparation of phenanthrenedione derivs. as CD45 inhibitors)
IT 604-95-5P 4733-06-6P 7473-71-4P 13292-03-0P
62896-78-0P 109313-55-5P 345630-35-5P 345630-37-7P
345630-38-8P 345630-40-2P 345630-42-4P 345630-43-5P
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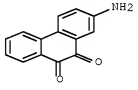
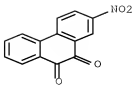
345631-38-1P 345631-39-2P 345631-40-5P 345631-43-8P
345631-44-9P
(preparation of phenanthrenedione derivs. as CD45 inhibitors)

L31 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:306240 HCAPLUS Full-text
DOCUMENT NUMBER: 135:70647
TITLE: Potent Reversible Inhibitors of the Protein Tyrosine Phosphatase CD45
AUTHOR(S): Urbanek, Rebecca A.; Suchard, Suzanne J.; Steelman, Gary B.; Knappenberger, Katharine S.; Sygowski, Linda A.; Veale, Chris A.; Chapdelaine, Marc J.
CORPORATE SOURCE: AstraZeneca Pharmaceuticals, Wilmington, DE, 19850, USA
SOURCE: Journal of Medicinal Chemistry (2001), 44(11), 1777-1793
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 02 May 2001
AB The cytosolic portion of CD45, a major transmembrane glycoprotein found on nucleated hematopoietic cells, contains protein tyrosine phosphatase activity and is critical for T-cell receptor-mediated T-cell activation. CD45 inhibitors could have utility in the treatment of autoimmune disorders and organ graft rejection. A number of 9,10-phenanthrenediones were identified that reversibly inhibited CD45-mediated p-nitrophenyl phosphate (pNPP) hydrolysis. Chemical efforts around the 9,10-phenanthrenedione core led to the most potent inhibitors known to date. In a functional assay, the compds. were also potent inhibitors of T-cell receptor-mediated proliferation, with activities in the low micromolar range paralleling their enzyme inhibition. It was also discovered that the nature of modification to the phenanthrenedione pharmacophore could affect selectivity for CD45 over PTP1B (protein tyrosine phosphatase 1B) or vice versa.
IT 36043-49-9P
(preparation and structure activity relationships of phenanthrenediones as inhibitors of protein tyrosine phosphatase CD45)
RN 36043-49-9 HCAPLUS
CN 9,10-Phenanthrenedione, 2-amino- (CA INDEX NAME)



IT 604-95-5P
(preparation and structure activity relationships of phenanthrenediones as inhibitors of protein tyrosine phosphatase CD45)
RN 604-95-5 HCAPLUS
CN 9,10-Phenanthrenedione, 2-nitro- (CA INDEX NAME)



CC 1-3 (Pharmacology)
Section cross-reference(s): 25
IT 604-94-4P 32155-34-3P 36043-49-9P 53622-33-6P
345631-41-6P
(preparation and structure activity relationships of phenanthrenediones as inhibitors of protein tyrosine phosphatase CD45)
IT 604-95-5P 607-09-0P 13292-03-0P 32060-67-6P
47194-23-0P 51789-39-0P 62896-78-0P 73671-07-5P 109497-01-0P
137354-59-7P 345224-95-5P 345224-96-6P 345224-97-7P
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346717-82-6P 346717-83-7P
(preparation and structure activity relationships of phenanthrenediones as inhibitors of protein tyrosine phosphatase CD45)
REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1922:15423 HCAPLUS Full-text
DOCUMENT NUMBER: 16:15423
ORIGINAL REFERENCE NO.: 16:2684h-i,2685a-i
TITLE: Amino- and anilinophenanthrenequinones
AUTHOR(S): Brass, Kurt; Ferber, Erwin
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1922), 55B, 541-56
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 16 Dec 2001
AB cf. C. A. 14, 3070. 2-Bromophenanthrenequinone (A), treated with PhNH2, PhNH2.HCl or 2PhNH2.H2SO4 under ordinary conditions, under pressure or in PhNO2 as a diluent, does not react with elimination of HBr, but the A acts as an oxidizing agent and the resulting dark blue to black products are substances closely related to aniline black. If they are freed from the

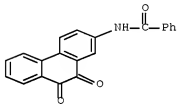
excess of PhNH2 and the unchanged A is removed with alkaline Na2S2O4, they can easily be oxidized to benzoquinone with CrO3; the 2-bromophenanthrenequinol (B) formed simultaneously, however, also reacts with any PhNH2 still present with the formation of phenylaminohydroxyphenanthrene. The same results are obtained when AcNHPh or its Na salt or the Na or Al salts of PhNH2 are used instead of PhNH2. The monophenylhyrazone of A does not react with PhNH2 in the desired sense, nor does the dibenzoate of B. Recourse was then had to the phenylation of aminophenanthrenequinones. 2- and 4-Nitrophenanthrenequinones are obtained in 20 and 13 g. yields, resp., by nitration of 30 g. phenanthrenequinone. The 2-NO2 compound (5 g.), rubbed to a thin paste with 250 cc. NaOH (d. 1.065), slowly treated with somewhat more than 4 mols. solid Na2S2O4, warmed a short time at 50°, diluted, filtered and treated with air, gives 3.6 g. of the 2-NH2 compound (C), also obtained in 3.9 g. yield from 5 g. of the NO2 compound in much H2O quickly treated with a solution of NaSH prepared from 1.6 g. NaOH, shaken 0.5 hr. in a tightly stoppered flask, diluted and treated with air; it seps. from H2O in slender black-violet needles, brown in transmitted light, sinters 205-10°, gradually softens but does not m. clear 300°, soluble in concentrated H2SO4 with red-brown, in H2SO4 diluted with 0.25 part H2O with cress-red, in fuming acid (20% SO3) with green color; acetyl derivative (D), obtained with Ac2O in boiling AcOH, red-violet needles from the red-brown solution in PhNO2, m. 324° (decomposition), soluble in concentrated H2SO4 with brown, in H2SO4-H2O (4 : 1) with red-brown, in fuming acid with green color, easily forms a yellow vat from which it is repptd. unchanged (passing through green) by air, dyes cotton a dirty salmon-red; benzoyl derivative, prepared with BzCl in hot C5H5N, flat brown-red spears from PhNO2, m. 297-8°, soluble in H2SO4 with green-brown color, forms a deep-yellow vat which dyes cotton a turbid light red. 2-Acetylamino-o,o'-diacetylphenanthrenequinol, from C in a little AcOH heated a short time with excess of Ac2O and then boiled about 0.5 hr. with Fe filings, fine white needles from EtOH-H2O, m. 228°, subliming in silky needles, gradually dissolves in concentrated H2SO4 with green color. 4-Aminophenanthrenequinone, obtained almost quant. from the NO2 compound with NaSH and subsequent treatment with air, violet-brown crystalline meal with metallic luster from H2O, black warty aggregates from 96% alc., softens 207°, does not m. 340°, easily soluble in the usual solvents with intense red, in concentrated H2SO4 with yellow-olive, in more dilute acid (4 : 1) with red-brown color. 2-Ethylaminophenanthrenequinone, from 1.7 g. D and 0.9 g. EtBr heated 5.5 hrs. at 180° in C5H5N in a sealed tube, poured into much dilute HCl, filtered and deacetylated by boiling 1.5 hrs. with 1 : 1 H3PO4, violet-black powder, soluble in hot AcOH, PhNO2 and C5H5N with brown color, seps. from PhNO2 in crystalline warts, has no m. p. 2-Anilinophenanthrenequinone, from equimol. amts. of C and PhBr, with a little Cu powder, heated 4 hrs. at 200° in C5H5N, black, almost insol. powder, soluble in cold concentrated H2SO4 with dirty brown color, forms a vat with very great difficulty in aqueous, easily in aqueous alc. suspension, has no m. p., is almost insol. in aqueous or alc. KOH. 2',4'-Dinitro-2-anilinophenanthrenequinone, obtained (together with some [(O2N)2C6H3-]2, m. 143°) from 1 mol. each of C and 2,4-(O2N)2C6H3Cl, with a little CaCO3 and Cu powder boiled 1.5 hrs. in PhNO2, brown spear- and table-like crystals from PhNO2, m. 280°, soluble in concentrated H2SO4 with brown color, forms a vat in alkaline Na2S2O4, does not react with o-C6H4(NH2)2, forms in cold aqueous alc. KOH a salt recognized by the intense red color imparted to the solution, gives 2,4-(O2N)2C6H3OH with K2Cr2O7-H2SO4 (no diphenic acid could be detected); 1 g. heated 1 hr. at 80° with 100 cc. of 10% KOH gives 2',4'-dinitro-2- anilinodiphenyleneglycolic acid, brown amorphous powder, has no m. p., soluble in concentrated H2SO4 with red-brown color, forms easily soluble alkali and insol. Pb, Cu and Ag salts. 2',4',6'-Trinitro-2-anilinophenanthrenequinone, from C and 1 mol. picryl chloride, with a little NaOAc and a trace of Cu powder, refluxed 3 hrs. in alc., sandy powder of small red-brown table-like crystals or a red to red-brown amorphous powder, m. 304-5°, soluble in concentrated H2SO4 with yellow-green color, repptd. unchanged

by H2O, forms a vat with alkaline Na2S2O4 but gives no quinoxaline with o-C6H4(NH2)2, oxidized by K2Cr2O7-H2SO4 to picramide, gives with aqueous KOH 2',4',6'-trinitro-2-anilinodiphenyleneglycolic acid, does not m., decomps. 300° (heated in larger amts. in an open test-tube it deflagrates explosively at 160°).

IT 860207-88-1P, Benzamide, N-(9,10-dihydro-9,10-diketo-2-phenanthryl)- (preparation of)

RN 860207-88-1 HCAPLUS

CN Benzamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)- (CA INDEX NAME)



CC 10 (Organic Chemistry)

IT 4733-06-6P, Acetamide, N-(9,10-dihydro-9,10-diketo-2-phenanthryl)- 4733-06-6P, Phenanthrenequinone, 2-acetamido- 109497-01-0P, Phenanthrenequinone, 4-amino- 860207-88-1P, Benzamide, N-(9,10-dihydro-9,10-diketo-2-phenanthryl)- 860207-88-1P, Phenanthrenequinone, 2-benzamido- 861321-00-8P, 9-Fluorenecarboxylic acid, 9-hydroxy-2-(2,4,6-trinitroanilino)- 861337-30-6P, Phenanthrenequinone, 2-anilino- 861349-60-2P, Phenanthrenequinone, 2-(2,4,6-trinitroanilino)- 861349-63-5P, Phenanthrenequinone, 2-ethylamino- 861350-08-5P, Acetamide, N-(9,10-dihydroxy-2-phenanthryl)-, diacetate 861350-08-5P, 9,10-Phenanthrenediol, 2-acetamido-, diacetate 861373-57-1P, 9-Fluorenecarboxylic acid, 2-(2,4-dinitroanilino)-9-hydroxy- 861798-82-5P, Phenanthrenequinone, 2-(2,4-dinitroanilino)- (preparation of)

L31 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1916:14053 HCAPLUS Full-text

DOCUMENT NUMBER: 10:14053

ORIGINAL REFERENCE NO.: 10:2583a-i,2584a-c

TITLE: Dyes derived from phenanthraquinone

AUTHOR(S): Mukherjee, Kshitish C.; Watson, Edwin R.

CORPORATE SOURCE: Dacca, Bengal, India

SOURCE: Journal of the Chemical Society, Transactions (1916), 109, 617-28
CODEN: JCHTA3; ISSN: 0368-1645

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

ED Entered STN: 16 Dec 2001

AB A study undertaken because of the close relationship of phenanthraquinone (A) to anthraquinone (B). The methods of introducing additional HO groups used in the (B) series failed, owing to the feebler resistance of the (A) series, but the methods used for the production of anilino derivs. (Ullmann, Ber. 34, 2174(1901), and D. R. P. 113,011) were applicable. Attempts to obtain vat dyes from acylamino derivs. were not encouraging. 15 g. fuming H2SO4 (SO3 =

70%) were added to 1.5 g. 2-hydroxyphenanthraquinone in a small stoppered bottle which was kept closed at 35-40° for 48 hrs.; the resulting acid was isolated as barium 2-hydroxyphenanthraquinonesulfonate, violet, soluble in boiling H2O, insol. in absolute alc. 3 g. 2,7-diacetoxyphenanthraquinone in 30 cc. HNO3 (d. 1.39) were warmed to 50-60° for 1.5 min. by immersion in boiling H2O, followed by immediately pouring into H2O, giving nitro-2,7-diacetoxyphenanthraquinone, yellow-brown prisms, does not m. 290°; boiled in HOAc containing a few drops H2SO4 it yields nitro-2,7-dihydroxyphenanthraquinone (C), brown, does not m. below 290°. (C), heated on the H2O bath with Sn and concentrated HCl, did not dissolve, but turned first deep brown and then light brown; then warmed first with aqueous FeCl3 solution and boiled with dilute HCl until ash-free it gave amino-2,7-dihydroxyphenanthraquinone, plates, does not m. 290°, insol. in organic solvents, soluble in alkalies with a brown color; triacetyl derivative, amorphous; diazotization and boiling gave 2,4(?),7-trihydroxyphenanthraquinone, red-brown, does not m. 290°, soluble in alkalies with a brown color; triacetate, red-brown microcrystals, m. about 280°. 2,7-Diaminophenanthraquinone, NaOAc, and Ac2O heated at 160° for 1 hr., mixed with an equal volume of HOAc, and poured into H2O, gave the diacetamino derivative, chocolate-brown crystals, does not m. below 295°. 1 g. dibromophenanthraquinone (D), from (A) in PhNO2 with Br (D. R. P. 222,206), when boiled with 35 cc. HNO3 (d. 1.42) for 0.5 hr. and the solution poured into H2O, gave dibromonitrophenanthraquinone, yellow needles, m. 244-5°; 1 g. (D), boiled 2 min. with 10 cc. fuming HNO3 (d. 1.51) and 1.5 cc. H2SO4 and poured into H2O gave bromodinitrophenanthraquinone, yellow needles, m. above 300°. 2-Nitrophenanthraquinone (1 g.), 0.6 g. Br, and 6 cc. HOAc at 140° for 2 hrs. gave bromo-2-nitrophenanthraquinone (E), red-yellow plates, m. above 300°. 1 g. 4-nitrophenanthraquinone treated with excess of Br at 110° in as little PhNO2 as possible gave the bromo derivative, yellow prisms, m. 224-6°; 1 g. 2,7-dibromophenanthraquinone, 10 g. PhNH2, and 0.25 g. Cu powder were boiled for 2.5-3 hrs., filtered hot, and poured into an excess of dilute HCl; the resulting blue-black 2,7-dianilinophenanthraquinone does not m. below 300° and dyes wool blue-black shades. Similarly (D) gives a bluish dianilinophenanthraquinone, does not m. below 300° and dyes wool greenish blue shades; (E) yielded 2-nitroanilinophenanthraquinone (F), blue-black, does not m. below 300°, dyes wool blue-black shades; 4-nitroanilinophenanthraquinone, black, does not m. below 300°, dyes wool blackish shades; dinitroanilinqphenanthraquinone, black, gives greenish black shades on wool; nitrodianilinophenanthraquinone, dyes wool in black shades. Dianilinophenanthraquinone, heated with 10 parts H2SO4 (d. 1.84) at 110-20° for 1 hr. gives a sulfonic acid which dyes faster, greener shades than the parent substance. Similarly, at 125-30° for 2 hrs. (F) gives a sulfonic acid which dyes chrome-mordanted wool in olive-green shades. 1 g. (D), 1 g. p-O2NC6H4NH2, 5 cc. PhNMe2, and a trace of Cu powder heated at 160° for 3.5 hrs. and poured into dilute HCl gave bromo-p-nitroanilinophenanthraquinone, reddish violet, does not m. 280°, does not dye wool. 1 g. (D), 1.5 g. (C6H4NH2)2, 2 g. fused NaOAc, 0.35 g. CuCl2, and 20 g. PhNO2 boiled for 2 hrs., precipitated with Et2O, washed with alc., and boiled with H2O gave dibenzidinophenanthraquinone, black powder, does not m., does not dye wool. 2-Aminophenanthraquinone and BzCl in PhNO2. at 100° for 20 min. gave the benzoyl derivative, pinkish needles, m. 295°; as a vat dye it gives pale pink shades on cotton; 2-phthalylaminophenanthraquinone, pale orange needles, does not m. 295°, dyes cotton pale yellow in the vat; 2-oxalylaminophenanthraquinone, red-brown needles, does not m. 295°, does not dye cotton.

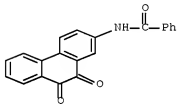
2,7-Dibenzoyldiaminophenanthraquinone, using BzCl in boiling PhNO2, brick-red needles, does not m. 295°, in the vat gives brown-orange shades on cotton; 2,7-diphthalyldiaminophenanthraquinone, brick-red needles, does not m. 295°, is not absorbed from the vat by cotton; 2,7-diaminophenanthraquinonesulfonic acid, using excess of fuming acid (SO3 = 70%) in a closed bottle for 48 hrs.

and pouring into H2O; in the moist state it dyes alummordanted wool dull green shades. Phenanthraquinonebisazophenol, diazotizing in 5% H2SO4 suspension, adding to a PhOH solution, and carefully making alkaline with Na2CO3, lenticular crystals, does not m. 295°, soluble in alkalies with a brown color; boiling with Ac2O and a drop of C5H5N and precipitating with alc. gives the acetate, brick-red prisms, m. 274°.

IT 860207-88-1P, Phenanthrenequinone, 2-benzamido-
(preparation of)

RN 860207-88-1 HCAPLUS

CN Benzamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)- (CA INDEX NAME)



CC 10 (Organic Chemistry)

IT 49546-41-0P, Phenanthrenequinone, 2,7-diamino-, diaceto derivative
860207-88-1P, Phenanthrenequinone, 2-benzamido-
860208-68-0P, Phenanthrenequinone, 2,4,7-trihydroxy-, triaceto derivative
860208-68-0P, Phenanthrenequinone, 2,4,7-trihydroxy- 860208-69-1P,
Phenanthrenequinone, 2-(phthalylamino)- 860208-70-4P,
Phenanthrenequinone, 2,7-dibenzamido- 860768-28-1P,
Phenanthrenequinone, 2,7-bis(phthalylamino)- 860768-29-2P,
Phenanthrenequinone, anilino-4-nitro- 871902-28-2P,
Phenanthrenequinone, 2,7-dianilino-
(preparation of)

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